#### **Nuclear Energy**

#### **NEAMS Reactor IPSC**

### Dave Pointer Technical Integrator, SHARP Reactor Integrated Performance and Safety Code Argonne National Laboratory

For the SHARP Development Team:

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Presented to NEAMS CT Workshop Marriott Chattanooga Convention Center April 4, 2011



#### **Reactor IPSC Goals and Strategy**

#### **Nuclear Energy**

### **★** Apply modern, high-performance computing techniques to nuclear reactor modeling

- Use advanced simulation tools to improve safety, reduce cost, explore advanced designs
- Provide local data needed to enable predictive fuel performance simulations
- Understand and reduce uncertainty of computational models

#### **★** Strategy

- Focus funding on reactor agnostic components to remain responsive
- Adopt multi-scale strategy to enable application to problems relevant to industry using a wide range of platforms
- Utilize modular architecture to enable component-wise use by most advanced users or integrated user interface driven application by less advanced users.
- Develop collaborations with customers to define near term applications/ demonstrations

#### **★** Customers

- Advanced Reactor Concepts
- Next Generation Nuclear Plant
- Light Water Reactor Sustainability
- Small Modular Reactors

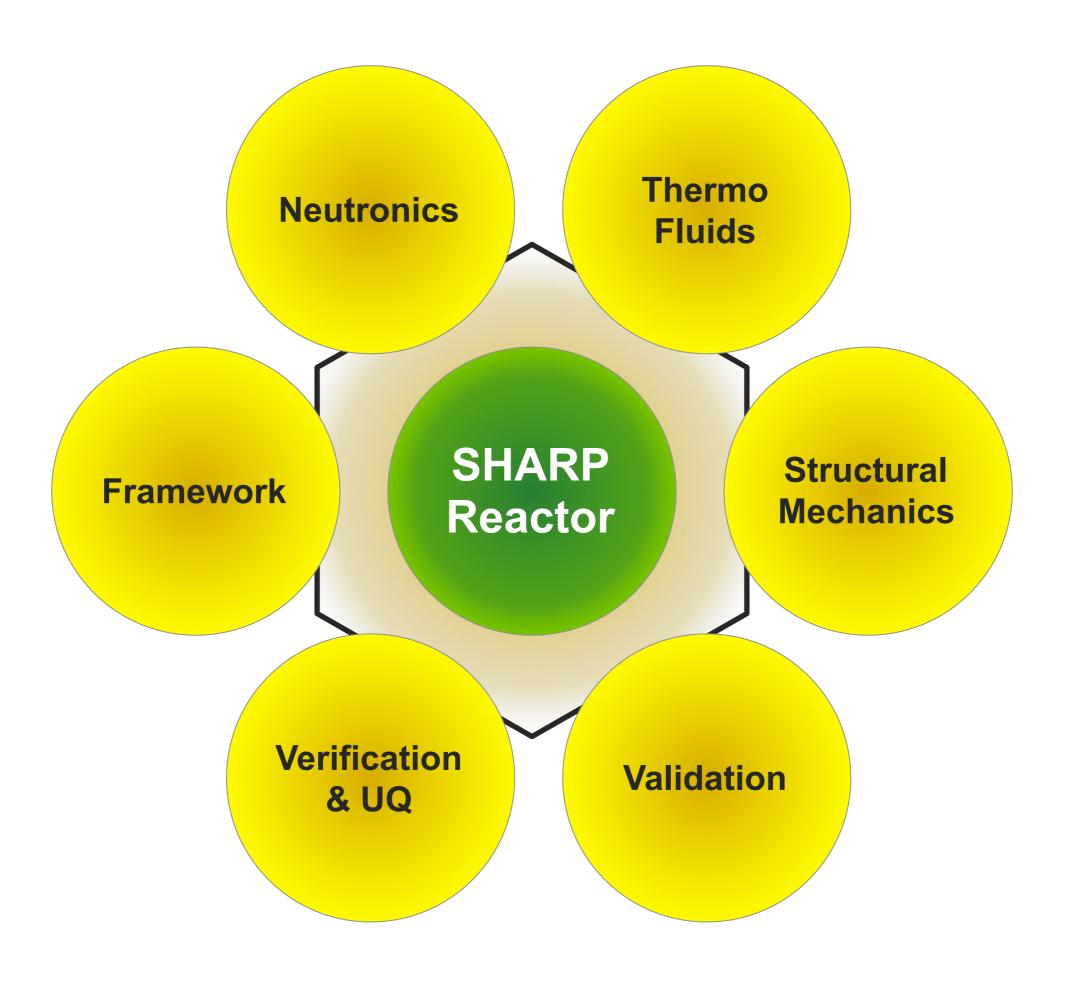


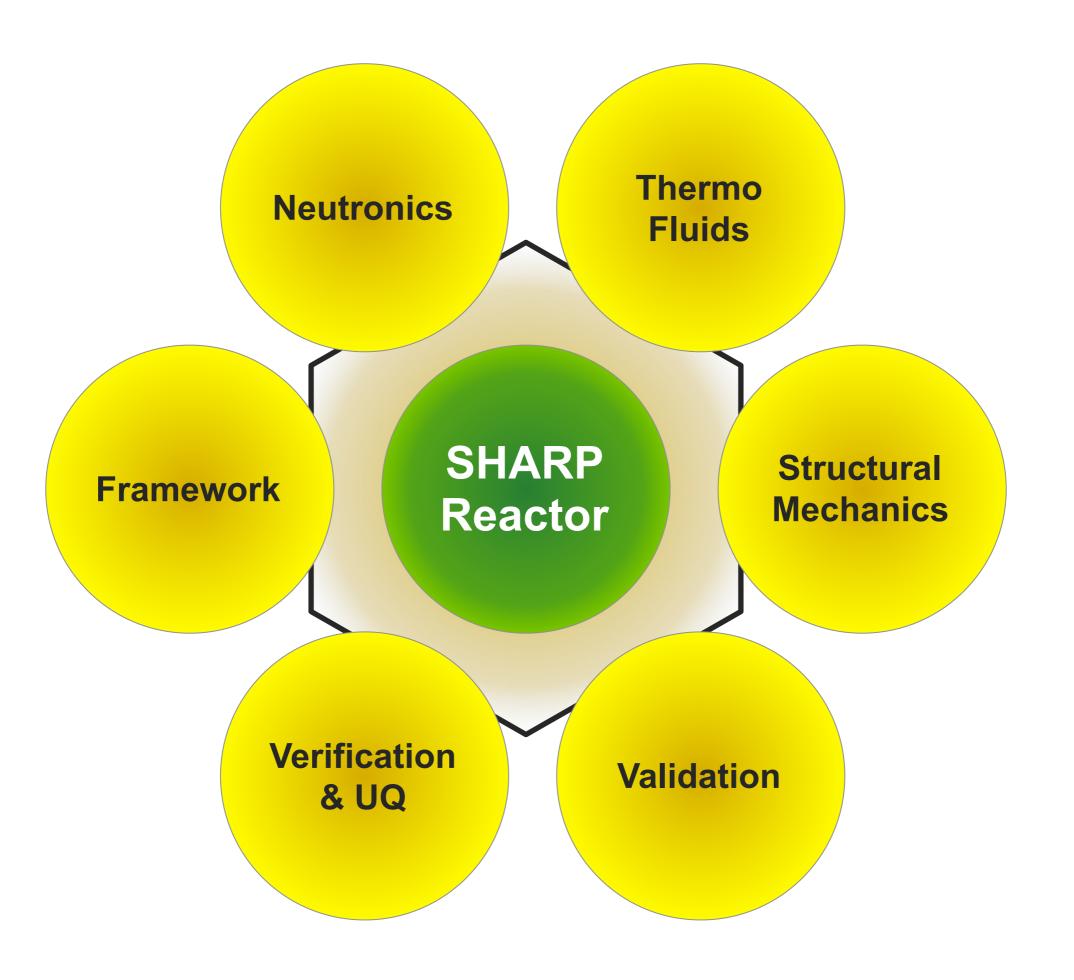


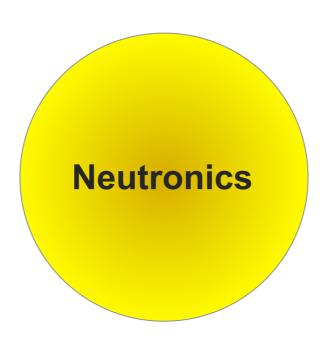
#### **Challenge Problems**

- ■Structural Mechanics Feedback for SFR Passive Safety
- ■Grid to Rod Fretting in LWR Fuel Assemblies
- Tenacious Crud Growth in Advanced BWR Fuel Assemblies
- Natural convection stability during SMR startup
- ■Thermal mixing in VHTR outlet plena











#### **Proteus Modules**

#### **Nuclear Energy**

**Neutronics** 

#### UNIC transport solver modules

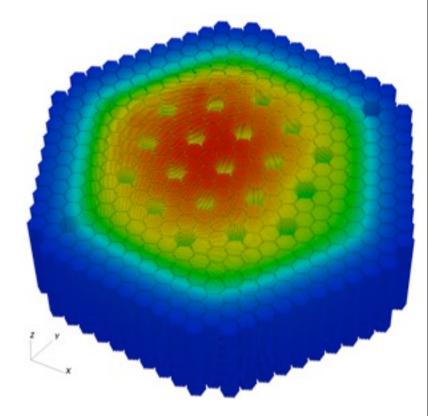
- MOC-FE provides 3-D & 2-D MOC
  - targeting problems with minimal homogenization
- SN2ND provides 1st and 2nd Order Discrete Ordinates
  - demonstrated from desktop to petascale platforms
  - prefer to homogenize pin cells
- PN2ND provide 1st and 2nd Order Spherical Harmonics
  - prefer to homogenize assembly internals
- NODAL provides a diffusion theory based structured geometry solver
  - fast running, highly scalable full core simulator

#### ■ MC<sup>2</sup>-3 module

 Provides high resolution cross-section libraries for fast spectrum applications

#### **■ MOCARV simulation module**

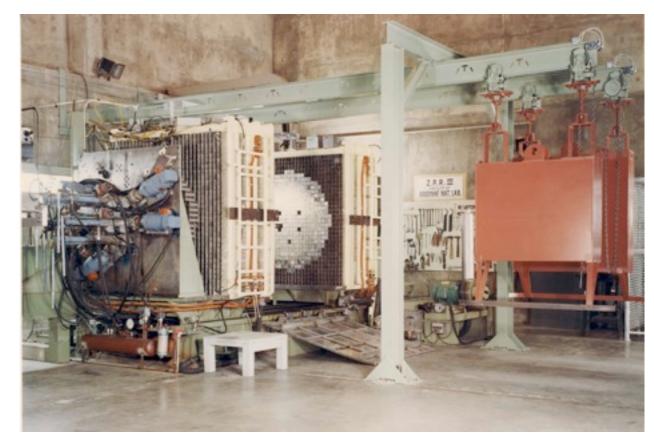
- Integrates 2-D MOC representations of radial planes with Sn Transport in axial direction
- Simulation modules to support reactor kinetic and fuel cycle analysis using the UNIC transport solver modules are in preliminary stages of development

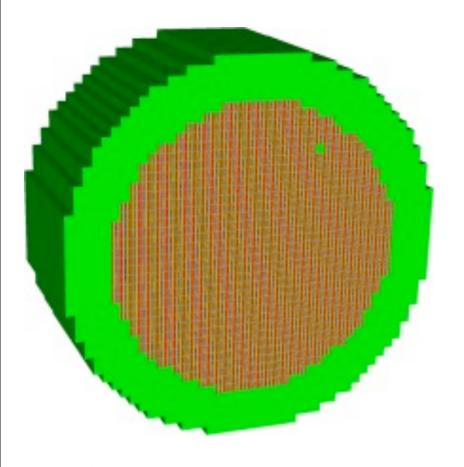


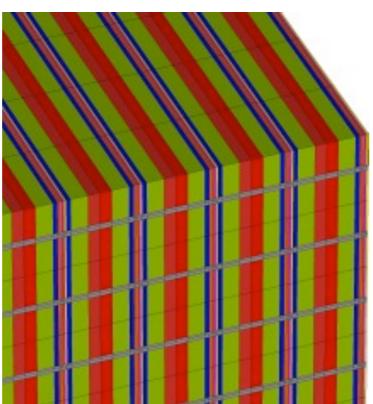


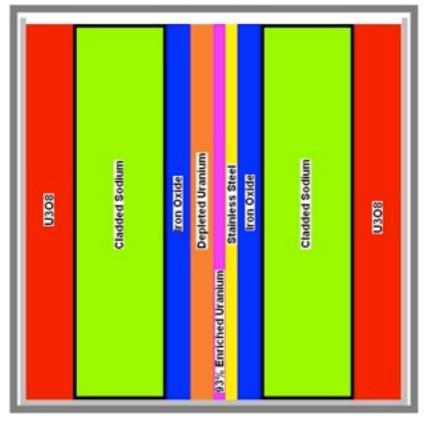
#### Example: ZPR6 Assembly 6A

- As part of a validation and performance study, we are modeling a well-documented reactor experiment (ZPR-6)
  - Development: 2·10<sup>6</sup> → +50·10<sup>6</sup> vertex mesh
  - 20 million vertices, 100 angles, 33 group calculation requires ~45 minutes on full Cray XT5 (~130 billion dof)



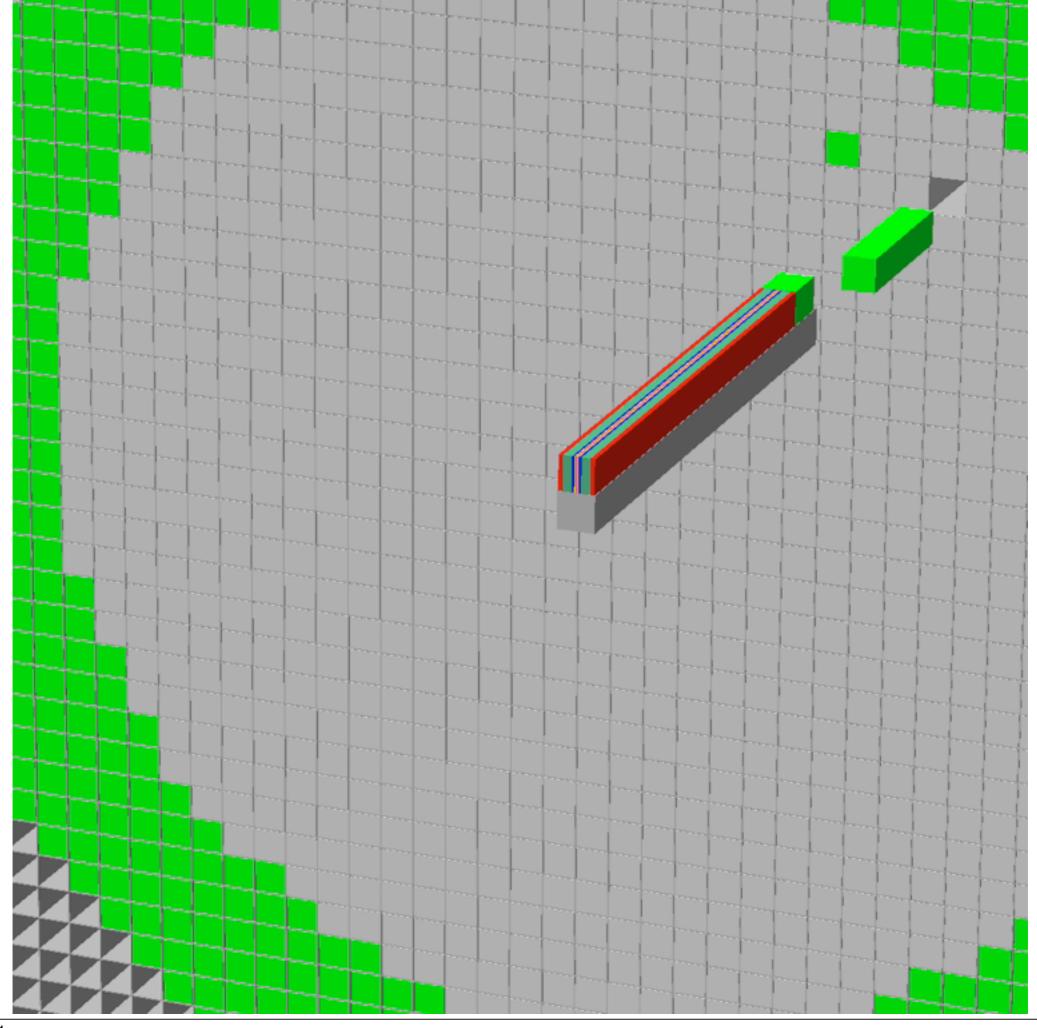






**Exact Geometry** 





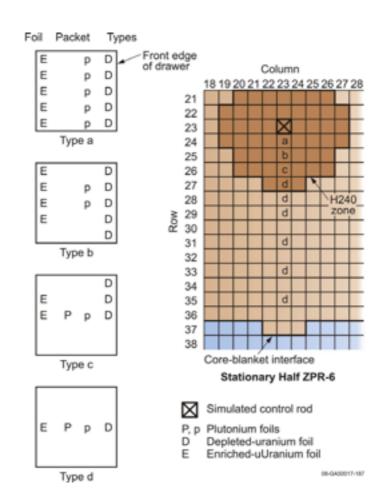


Stationary

#### **Nuclear Energy**

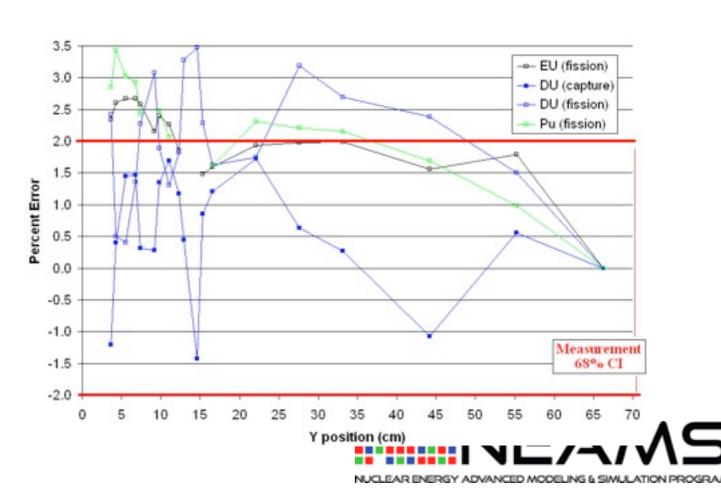
# Empty Matrix Tubes DU Blanket Filled Tubes Inner High Pu240 Zone Sodium Filled Drawer Outer Pu Drawers Insertion Safety Rods DP Drawer Locations Fission Chamber Location Autorod Location

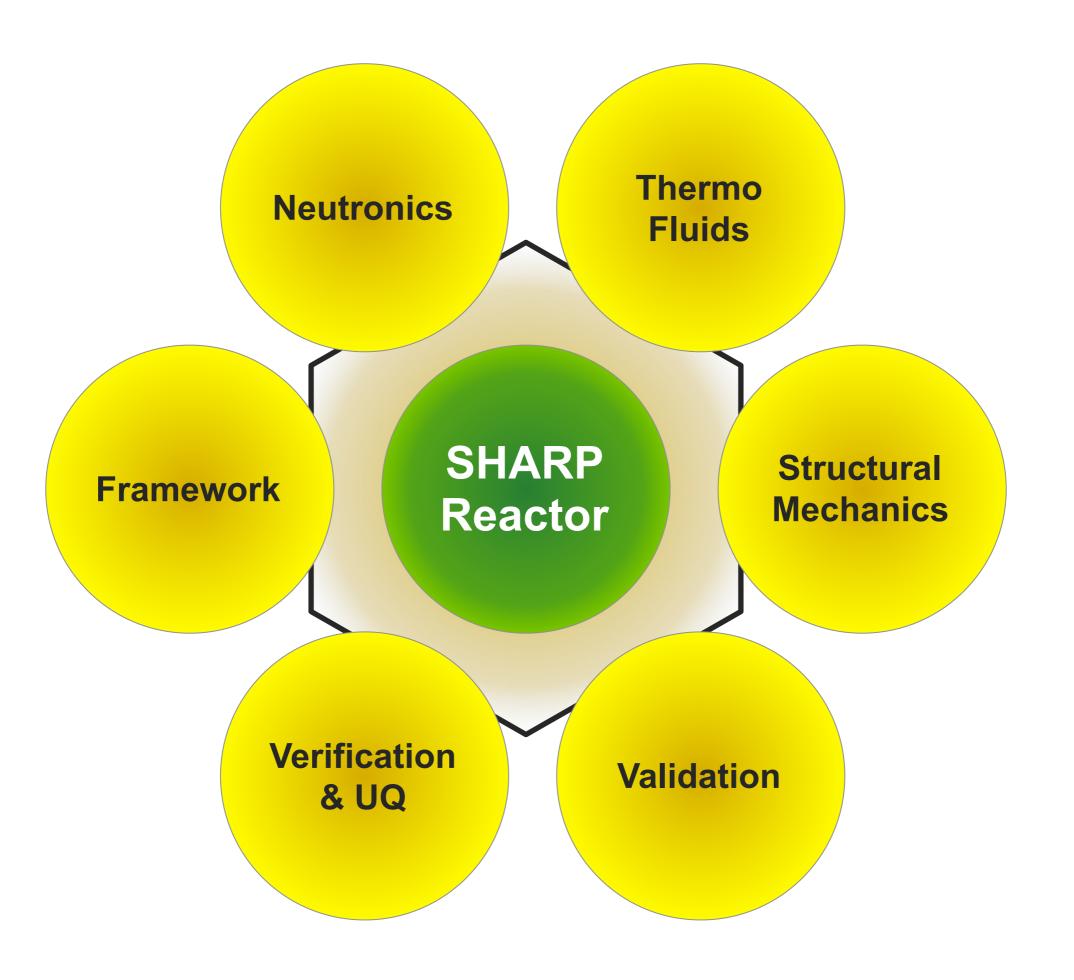
Movable

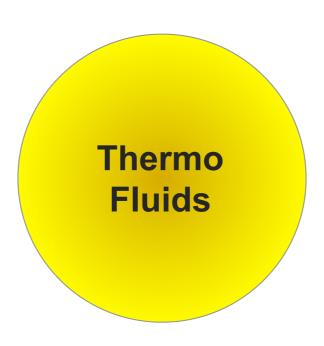


### Flux Solution for ZPR6 Assembly 6A Experiments

- ZPR6/7 Loading 104 consists of a Pu filled core with a High Pu240 central core region.
  - In loading 104
    - fuel removed from the center drawer to simulate an open control rod position
    - foil measurements were carried out to investigate the altered energy dependence with respect to the other loadings.
- Predictions are shown below with 2% experiment confidence interval in red.
- The result is considered excellent compared with legacy approaches.
- **■** Enables development of truly predictive fuel performance codes









#### **SHARP-TH Modules**

#### **Nuclear Energy**



#### ■ Nek5000 DNS/LES module

- highly-scalable, high-order spectral element CFD
- direct Numerical Simulation
  - solves for stress tensor directly
  - limited to small regions because very high resolution mesh is needed
- large Eddy Simulation
  - uses spectral filtering or sub-grid model for smallest turbulence length scales
  - applicable to component analysis

#### ■ Nek5000 URANS module

- solves Unsteady Reynolds Averaged Navier Stokes equation using two to six equation closure models to approximate turbulent stresses
- applicable to large regions

#### ■ STAR-CCM+ module

- provides access to steady and unsteady RANS solvers of STAR-CCM+
- applicable to large regions, up to full core
- provides access to STAR-CCM+ steady state eulerian-eulerian multiphase solver

#### ■ SHARP-IF module

- intermediate fidelity simulation toolset using momentum sources to mimic effects of geometric details
- applicable to full core +

#### ■ SAS11 modules

- lumped parameter representation of T/H and Structural Mechanics applicable to full system
- provides continued access to legacy SFR fuel performance models





#### **Nuclear Energy**

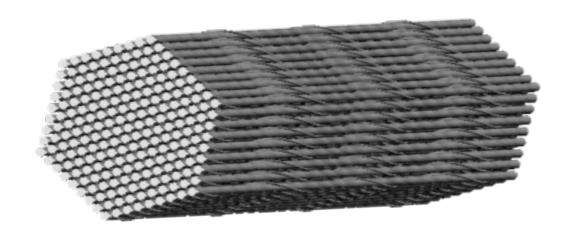
### Key Findings: CFD Simulations of SFR Assemblies

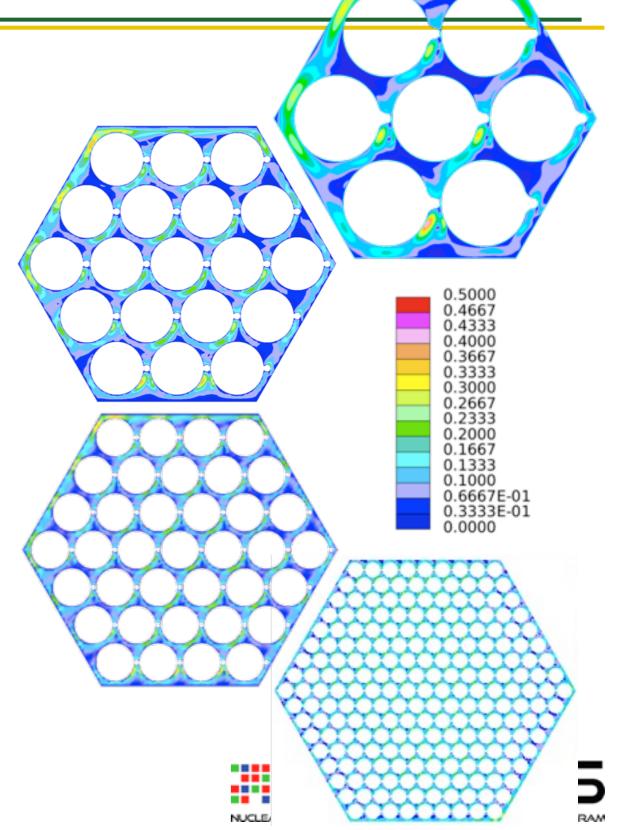
7-217pin wire-wrapped assemblies

D. Pointer, P. Fischer, A. Obabko, E. Merzari, R. Hu Argonne and J. Smith, UWisc

#### Demonstrated evolution of flow field from 7 to 217 pin assemblies

- Reduced importance of bulk swirling and increased complexity of flow field with increasing pin count
- Fundamental change in flow behavior between 19- and 37-pin assemblies
  - Important because most experiments have been completed using 19 pins
  - Explains observations in small number of experimental pressure drop data sets for large bundles





RANS-based CFD

LES

LES



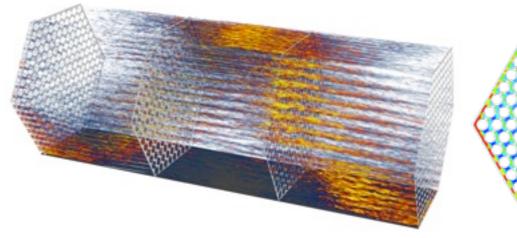
#### **Nuclear Energy**

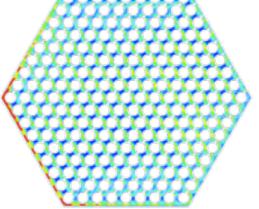
#### Key Findings: Core Flow Analysis

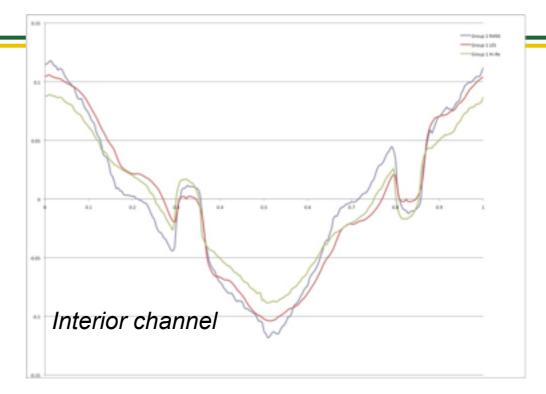
217pin wire-wrapped assemblies P. Fischer, A. Obabko D. Pointer, and J. Smith

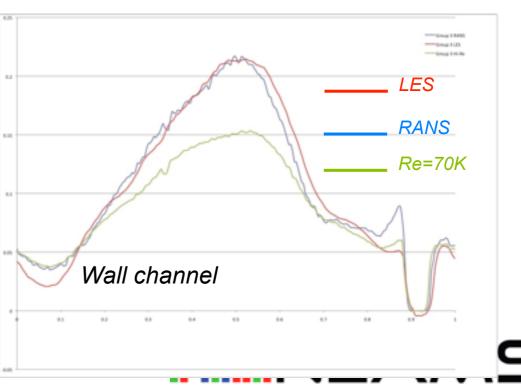
#### 217 pin analysis –

- Good agreement with very limited data available from large assembly experiments completed at HEDL.
- Detailed assessment of cross flow in large bundles
- Demonstration that Reynolds number effects are isolated to the edge channels
- Confirmation that RANS methods are applicable in real geometry
- 30 M CPU hours provided by DOE INCITE program





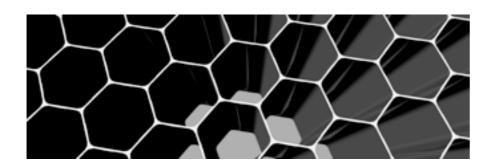




Hydrodynamic Analysis of Different Spacing Strategies for a Tight-Lattice SFR bundle

#### **Nuclear Energy**

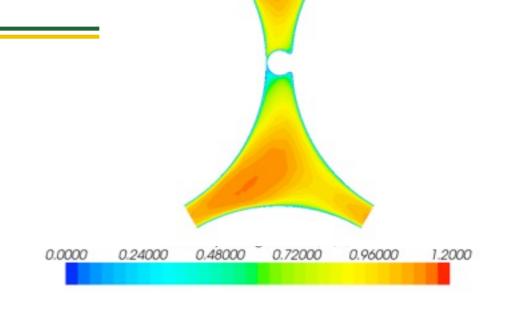
- > Comparison between spacer grids and wire wrappers for P/D =1.08
- > Spacers lead to considerably higher pressure losses (2.5 times the value of the bare bundle case)



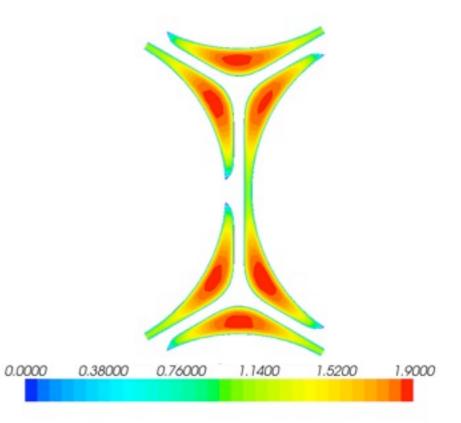
Bare (Cheng- Todreas)	Bare (CFD)	Wire (Cheng- Todreas)	Wire (CFD, Reynolds Similarity)	Wire (CFD, Matched Mass Flow)	Spacer Grid (CFD Matched Mass
0	+8%	+45%	+24%	+46%	+>150%

Comparison between the computed pressure drop as a percentage difference to the bare bundle prediction of the Cheng-Todreas correlation..

Building searchable bibliography of SFR fuel assembly experiments with key flow and heat transfer parameter database fields.

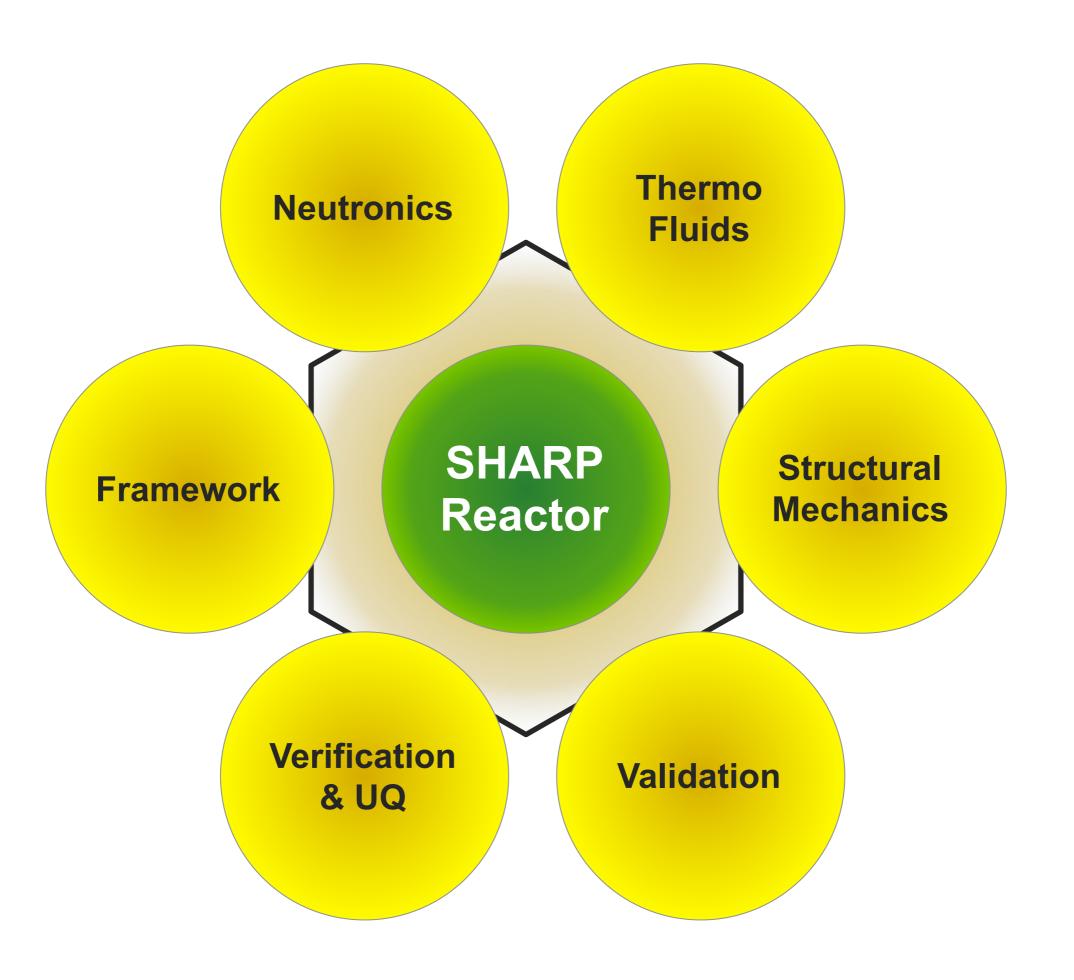


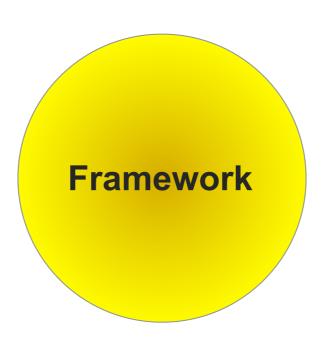
RANS-based CFD



Identical mass flow rate.

E. Merzari, J. G. Smith and W.D. Pointer, "Hydrodynamic Analysis of Different Spacing Strategies for a Tight-Lattice SFR bundle," accepted for publication at 2010 ANS Winter Meeting, Las Vegas, NV







#### **SHARP Framework Modules**

#### **Nuclear Energy**

**Framework** 

#### **■ MOAB** module

- highly scalable data management for mesh based simulations
- Currently integrated into UNIC, Nek5000, Star-CCM+ and DIABLO

#### ■ MB Coupler module

scalable parallel solution transfer between meshes of different types

#### ■ MeshKit Modules

- MeshKit Generation Library
  - Provides consistent API access mesh generation functionalities in MeshKit or other libraries
  - Includes RGG reactor geometry/meshing tool
- CGM Geometry Library
  - Library for CAD and other geometry types
  - Includes interface to Open.CASCADE, an open-source library for geometry
  - compatible with (and can import models from) CUBIT's CGM
- Lasso relations library
  - Allows associate of mesh to geometry without requiring software dependency between mesh and geometry libraries





#### SHARP Framework: Solution Transfer

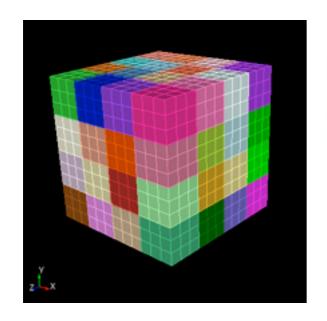
#### **Nuclear Energy**

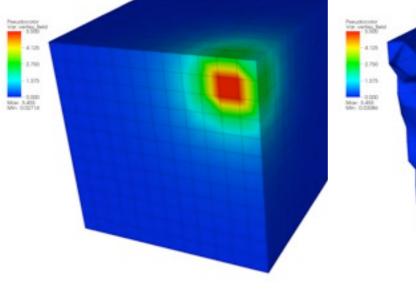
#### General approach

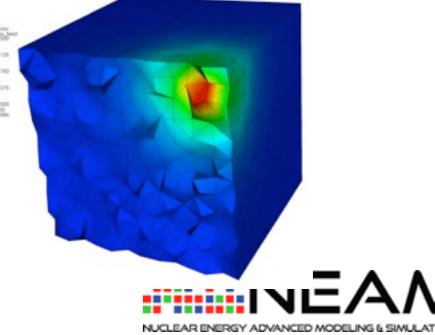
- -Solution & mesh stored in iMesh instance on each processor
- -Two meshes can be disjoint & distributed independently
- -Overall structure is similar whether you're coupling between FD, FEM, SEM
- -Results can be used for both operator-split and higher-order coupling

#### Coupling steps:

- Initialization (parallel mesh read, initialize kdtree search structure)
- -Point location (locate target points/mesh in source mesh)
- -Interpolation (project solution onto target points/mesh)
- -Normalization/conservation





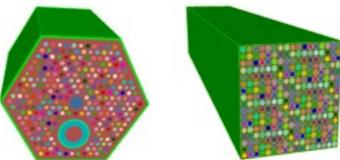


### SHARP Framework: Mesh Generation Tool for Lattice Hierarchy-Based Reactor Core Geometries and Meshes

- MeshKit (A tookit based on ITAPS libraries, developed at Argonne National Lab).
- MeshKit's RGG (Reactor Geometry Generator) has two tools:

#### 1. Assygen -

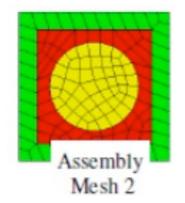
- It generates assembly geometry and meshes based on an text input file description.
- Supports rectangular and hexagonal assemblies.

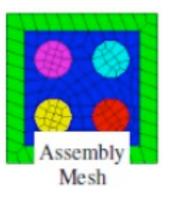


#### 2. Coregen -

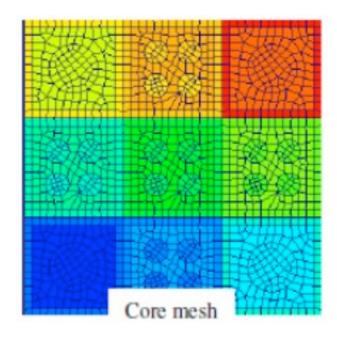
- Assembles assembly meshes by copy/ move and merge assembly meshes.
- It supports full rectangular and 1/6, 1/12, full hexagonal assemblies.

Assygen uses text input files to create assembly geometry and meshes using CUBIT.

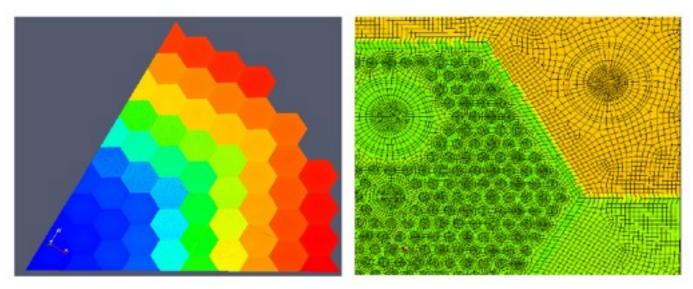




These meshes are copy/move/merge 'd to create a full rectangular core.

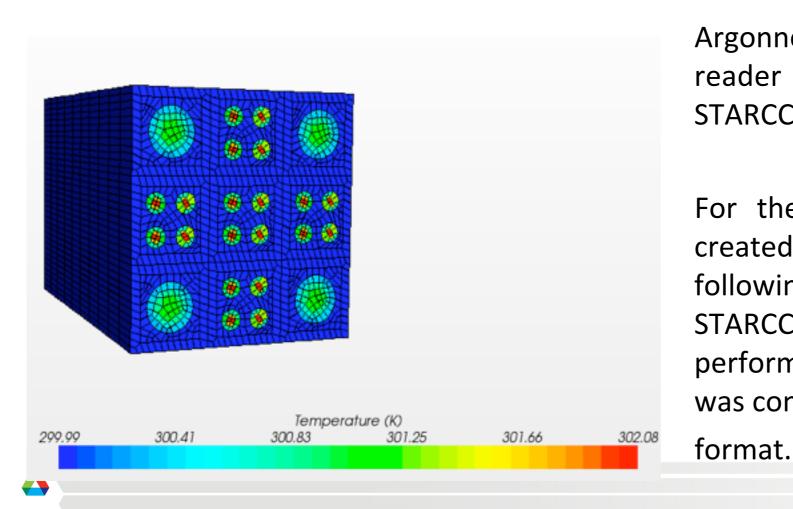






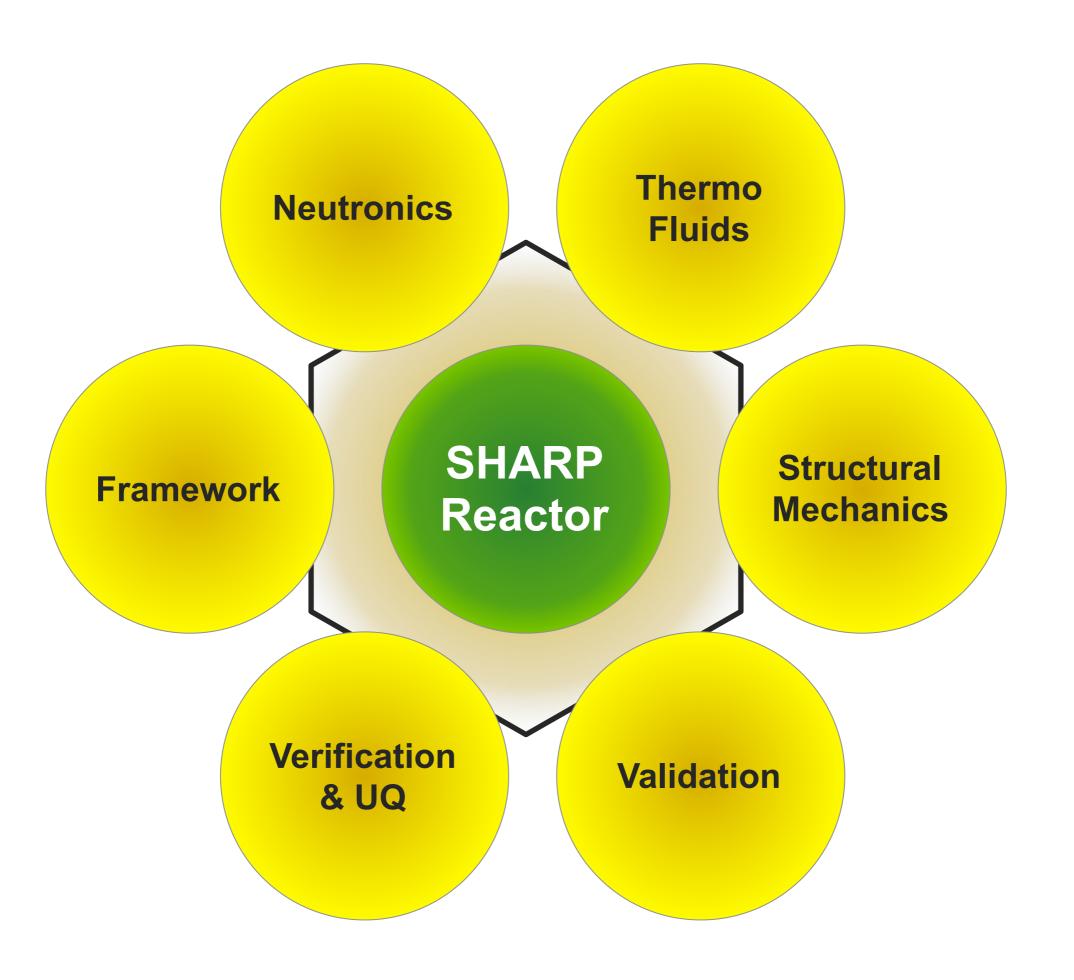
Sixth of a VHTR core with 12M hexes took 4 min for creating assembly geometry; 4 min for meshing using Cubit and 23 min for copy/move/merge assemblies to form the reactor core.

#### STARCCM+ reader and writer



Argonne's iMesh implementation MOAB has reader and writer for converting to/from STARCCM+ meshes to other mesh formats.

For the toy example in the previous slide created by using 'Assygen' and 'CoreGen' the following mesh was successfully imported by STARCCM+ and simple test calculations were performed. MOAB native file format (.h5m) was converted to STARCCM+ (.ccm/ccmg) file .



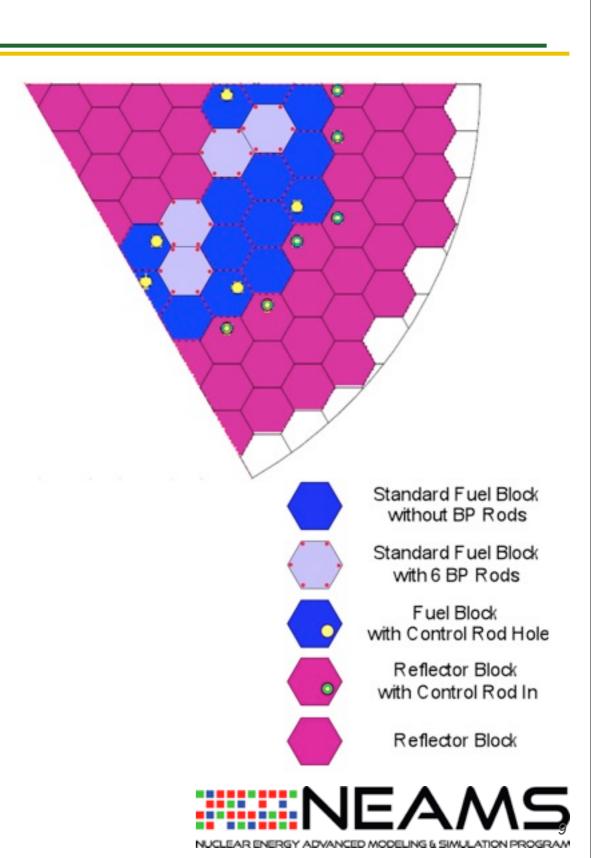




#### Integrated Multiphysics VHTR Analysis

Neutronics, TH, and Framwork

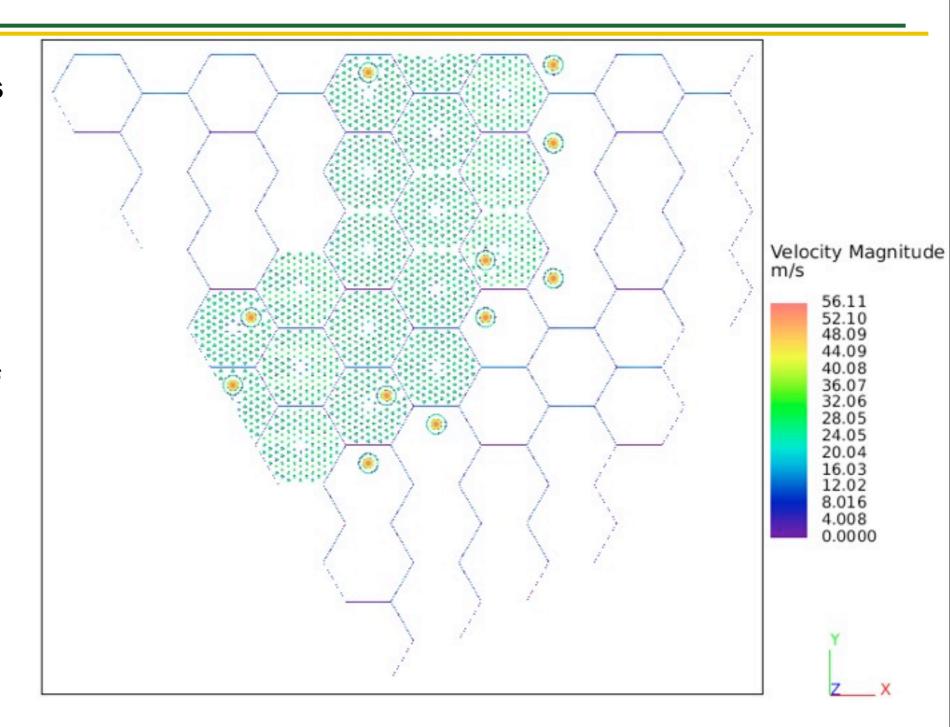
- Benchmark model based on GT-MHR
- Core Layout
  - 60° periodic boundaries
  - 3 rings of fuel columns
  - Control rod channels open in fuel columns
  - Control rods fully inserted into reflector columns ("operating rods in")
- Burnable poisons biased towards inner ring to flatten power shape
- All fuel enrichment is 10.5%
- Average power density 29 MW/m³
- Relatively coarse mesh to reduce computation expense





#### **Predicted Core Flow Distribution**

- Inlet mass flow rate is assumed to be 289.9 kg/s
- **■** Predicted flow splits
  - 75% through coolant channels
  - 25% through bypass
    - 10% between blocks
    - 15% in control rod holes



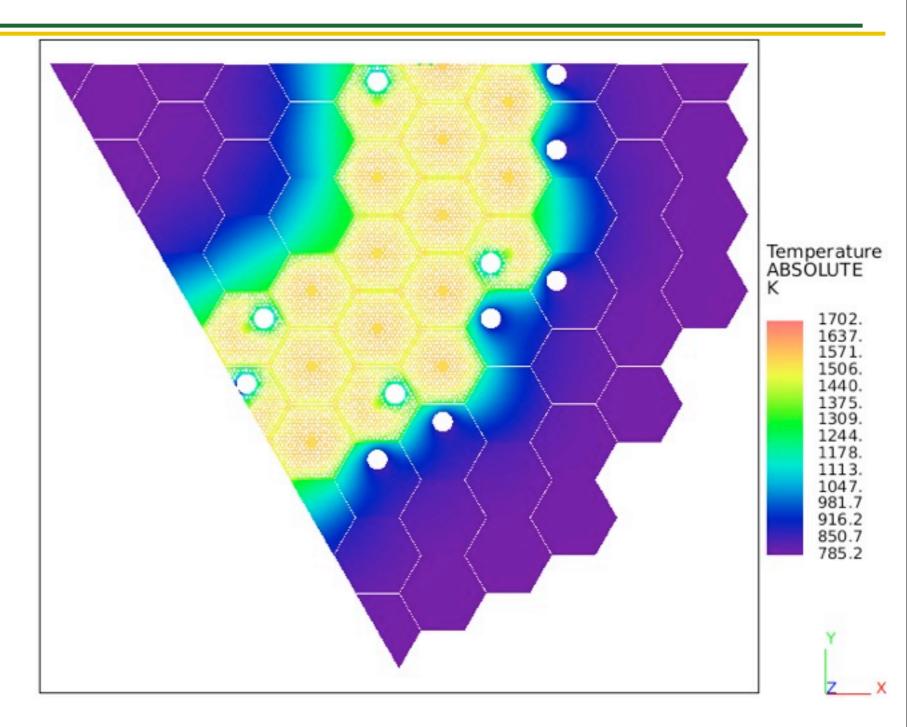




#### Results of Stand Alone CFD Simulations with Flat Power Profile

#### **Nuclear Energy**

Effects of bypass coolant flow paths are clearly visible in the predicted graphite temperature

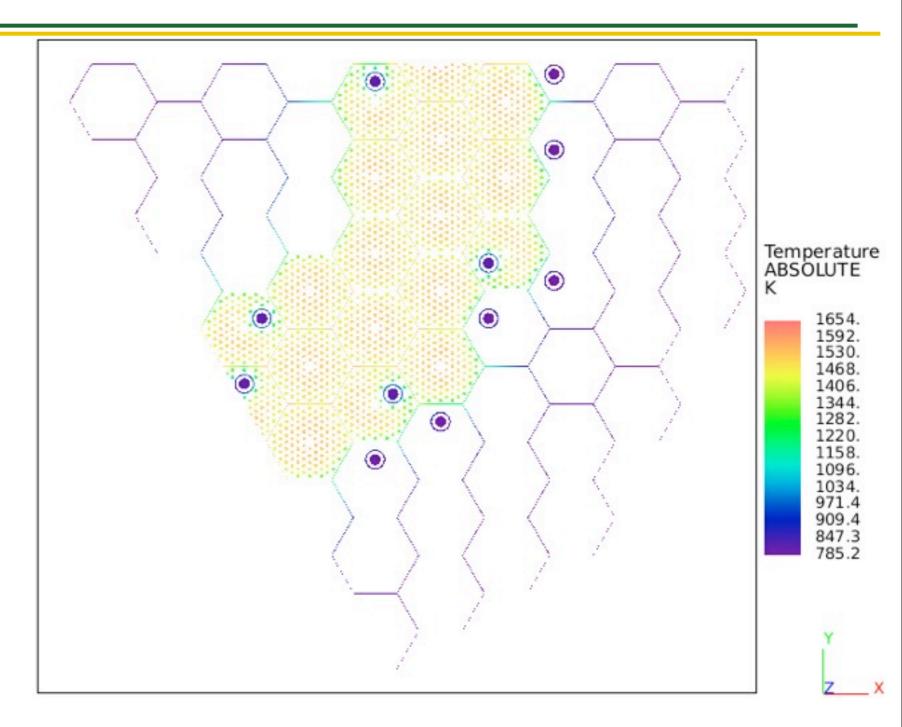




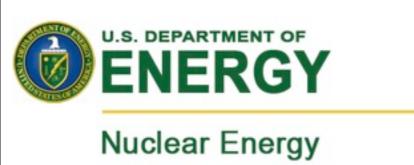


### Results of Stand Alone CFD Simulations with Flat Power Profile

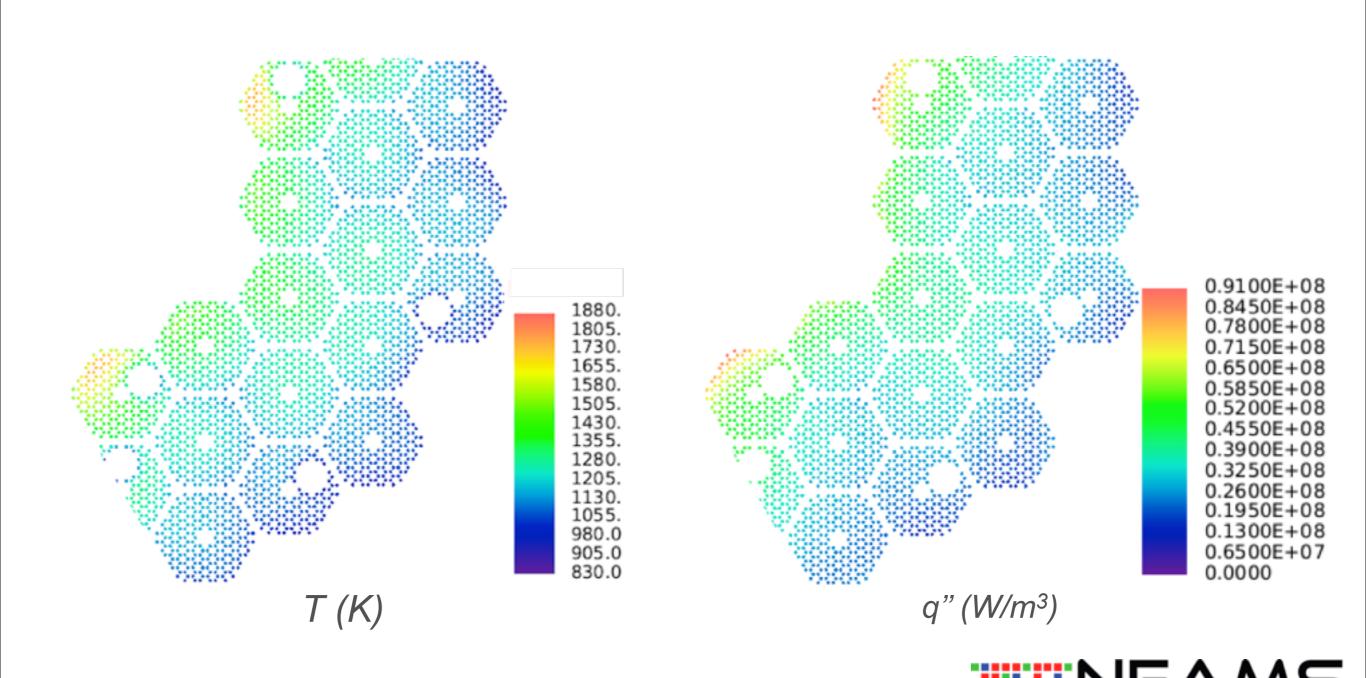
- Little radial mixing occurs within the bypass gap flow, and coolant temperature rise is primarily isolated to the fueled annulus
- Peak coolant temperatures occur in the gap bypass flow.

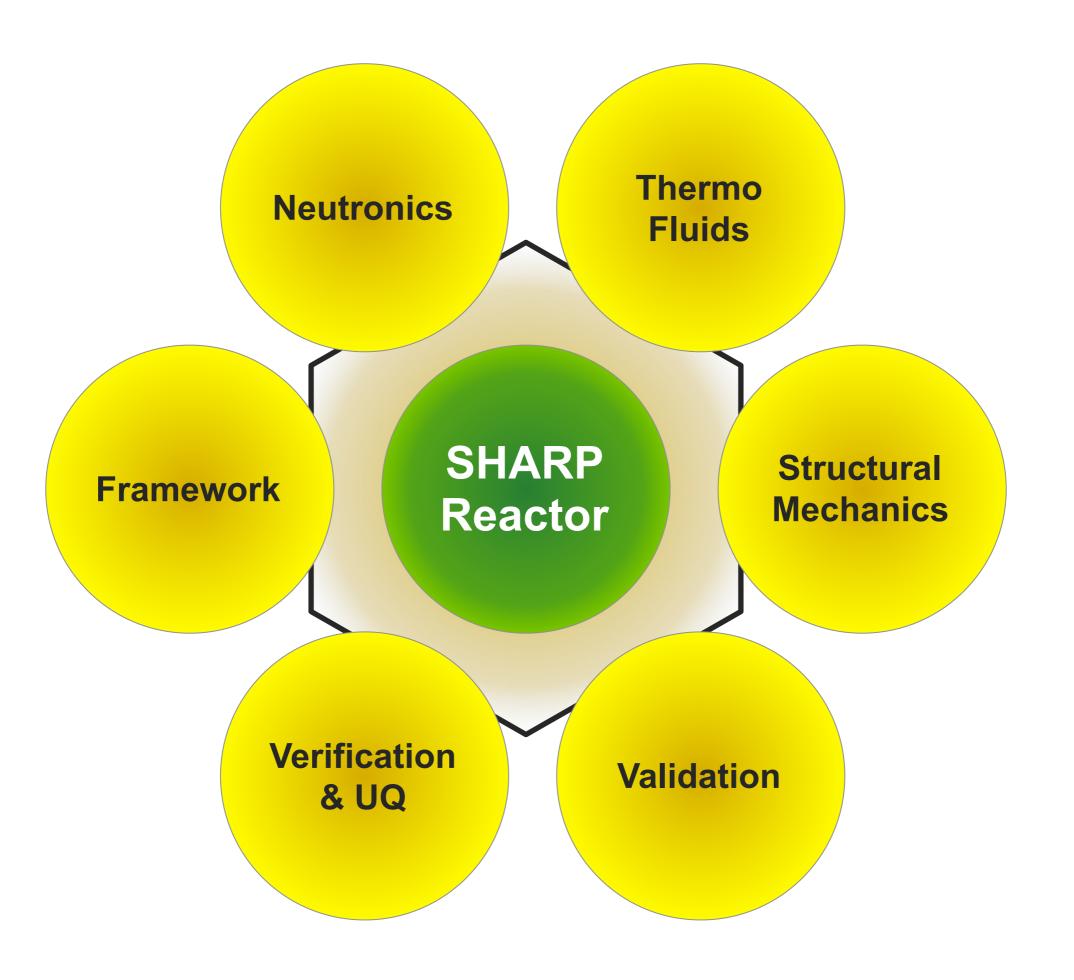






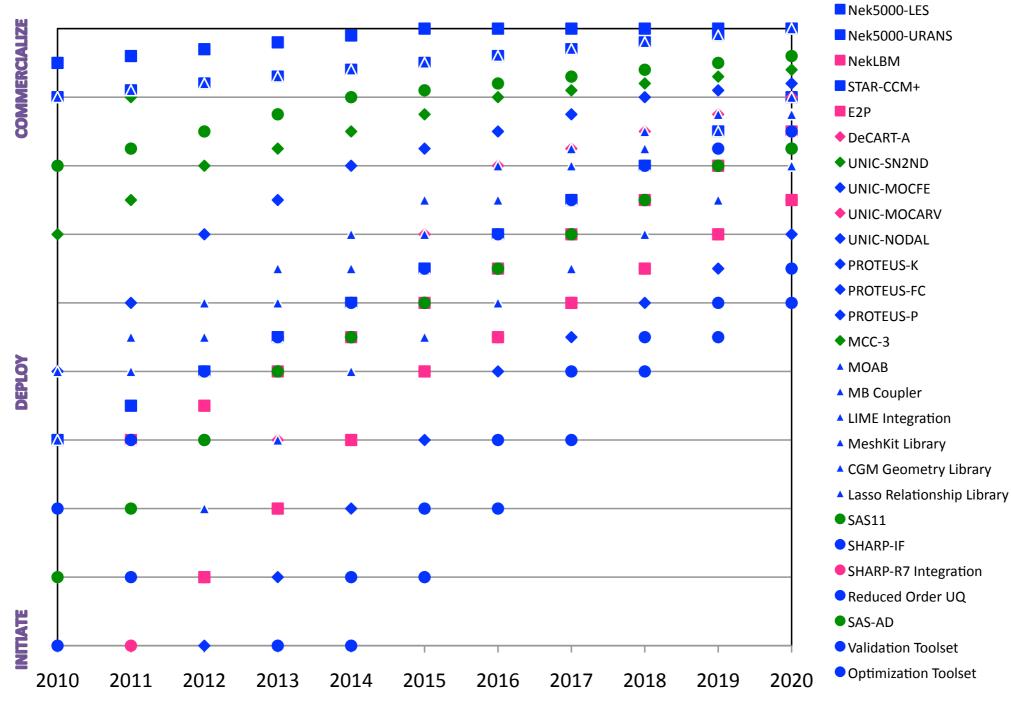
## FY10 Integrated Multiphysics VHTR Analysis: Radial Profiles at Outlet







#### Long Term SHARP Deployment Plan





#### **FY11 Successes and Plans**

#### **Nuclear Energy**

#### ■FY11 Budget - \$5.6M (~\$1.1M available under CR)

#### ■FY11 Successes

- Released version 4 Nek5000 module as open source toolkit
  - download at nek5000.mcs.anl.gov
- Released version 4.0.1 MOAB framework module as open source toolkit
  - download at trac.mcs.anl.gov/projects/ITAPS/wiki/MOAB
- Completed implementation of MC<sup>2</sup>-3 cross-section module
  - preparing for initial release

#### ■FY11 plans

- Reviewing mission and requirements
  - planning summer workshop with stakeholders to revise requirements
- Completing implementation of SN2ND module
  - preparing for initial release
- Completing initial coupling of DIABLO structural mechanics modules to SHARP framework
- Defining collaborations with CASL and RELAP7 teams

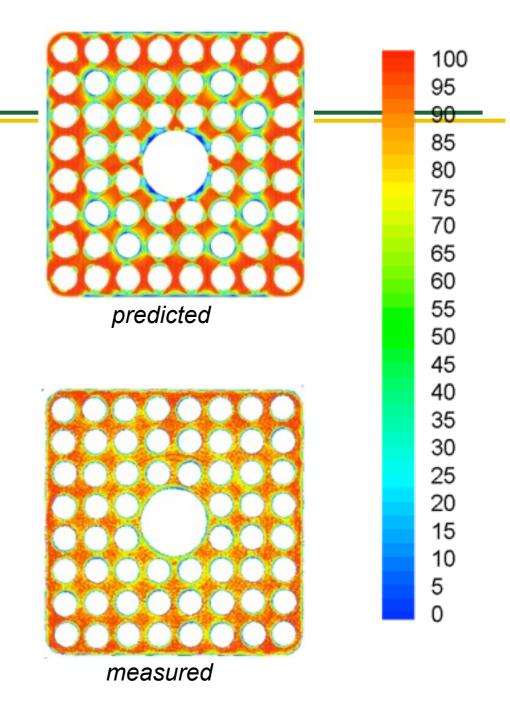




#### **Summary**

#### **Nuclear Energy**

- Module development efforts moving forward as a group
  - Tools are targeting multiple reactor types
    - roughly 70% of effort is reactor agnostic
  - Coupling taking place in many ways
    - Multi-physics
    - Multi-resolution
    - Multi-scale
- Continuous efforts in validation for each physics area
  - Includes development of data collection methods and methods for comparison of very large data sets



Prediction of Exit Void Fraction Distribution in an Electrically Heated Full Size BWR Fuel Assembly Using Extended Boiling Framework Developed as an Extension of STAR-CD (OECD/NRC BFBT Benchmark)

